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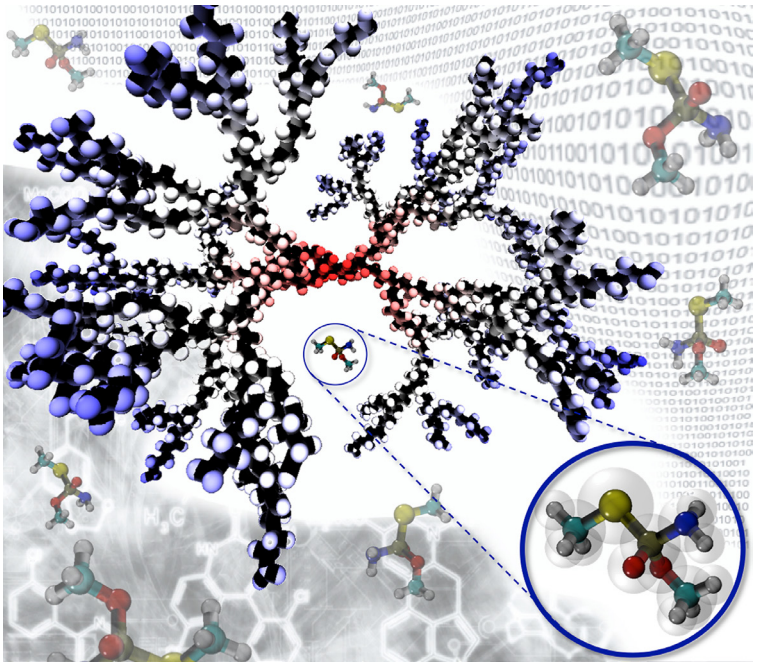
Cover Picture



Comparative *in-silico*/experimental study of functionalized dendrimers for nano-detoxification of organophosphate agents. The rational design of these nanoparticles allows increase their affinity and ability to capture organophosphates. Details are presented in the Article **Nano-Detoxification of Organophosphate Agents by PAMAM Derivatives** by *Esteban F. Durán-Lara, Fabian Ávila-Salas, Sebastian Galaz, Amalraj John, Adolfo Maricán, Margarita Gutiérrez, Fabiane M. Nachtigall, Fernando D. Gonzalez-Nilo and Leonardo S. Santos* on page 580.

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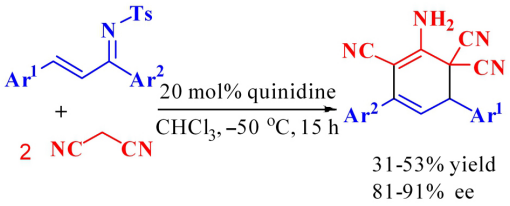
Editorial

403 **Who is Reading and Who is Citing the JBCS?**
Joaquim A. Nóbrega and Watson Loh

Communication

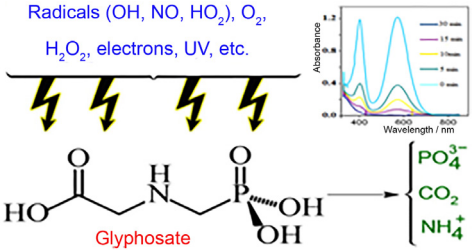
405 **Asymmetric Synthesis of Highly Functionalized Cyclohexa-1,3-dienes via Organocatalyzed One-Pot Three-Component Domino Reaction of Malononitrile with α,β-Unsaturated Imines**
SI online
Wei Chen, Ren-Zun Zhang, Xiao-Yan Lu and Jian-Wu Xie



Graphical Abstract
The enantioselective synthesis of highly functionalized cyclohexa-1,3-dienes was achieved via an organocatalytic one-pot three-component domino reaction

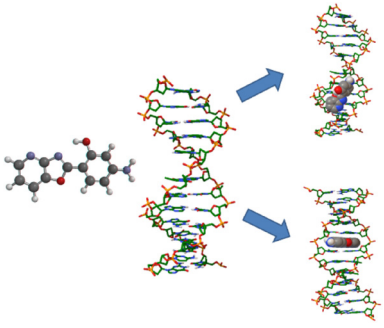
Articles

411 **Non-Thermal Plasma Induced Total Mineralization of Glyphosate in Water in the Presence of Iron II Ions**
Moïse Fouodjouo, Samuel Laminsi, Georges Y. Kamgang, Michele T. Mengue and Nito A. Debacher



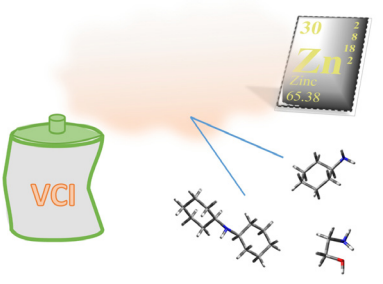
Graphical Abstract
Glidarc plasma completely mineralized glyphosate into CO_2, NH_4^+ and PO_4^{3-}. The kinetics has been studied and a plausible degradation pathway has been proposed

420 **Investigation of the Interaction of 2-(2'-Hydroxyphenyl)-benzoxazoles and their Derivatives with B-DNA by Docking and Molecular Dynamics**
SI online
Fábio dos S. Grasel, Tiago E. de Oliveira and Paulo A. Netz



Graphical Abstract
Quantum calculations, docking and molecular dynamics simulations were performed, analyzing the interactions between six 2-(2'-hydroxyphenyl)-benzoxazoles derivatives and the dodecamer d(CGCGAATTCGCG)$_2$. They showed favorable interactions, without DNA denaturation, and may act as potential biological probes

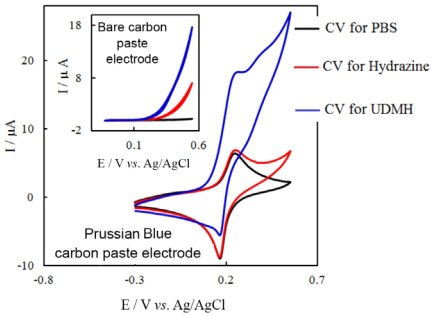
434 **Experimental and Theoretical Studies of Volatile Corrosion Inhibitors Adsorption on Zinc Electrode**
Deiver A. Teixeira, Marco A. G. Valente Jr., Assis V. Benedetti, Gustavo T. Feliciano, Sebastião C. da Silva and Cecílio S. Fugivara



Graphical Abstract
Amine-based volatile corrosion inhibitors (VCI) are adsorbed on Zn surface under a VCI positive vapor pressure environment, and the adsorbed inhibitors are easily removed by opening the container having the pieces, saving costs and time to clean the metallic surface

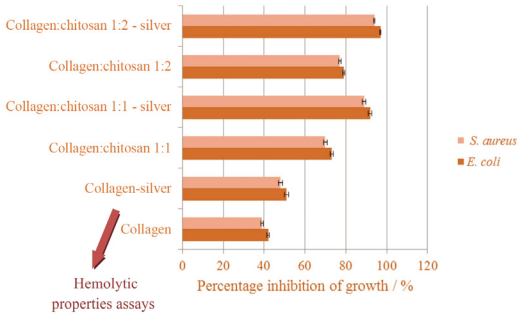
451 **Selective Determination of Unsymmetrical Dimethylhydrazine on a Prussian Blue Modified Carbon Paste Electrode**
Bagher Sobhanmanesh and Mostafa Najafi

Graphical Abstract
This paper describes a carbon paste electrode modified with Prussian Blue for selective determination of unsymmetrical dimethylhydrazine (UDMH) in the presence of hydrazine



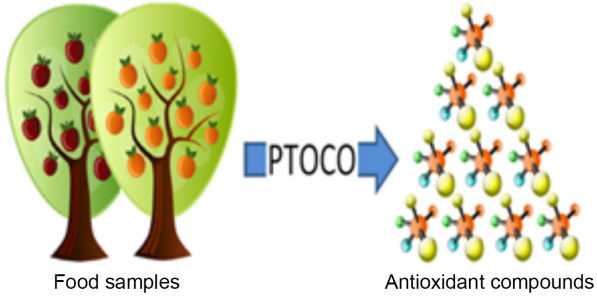
458 **Improving Natural Biopolymeric Membranes Based on Chitosan and Collagen for Biomedical Applications Introducing Silver**
Camelia Ungureanu, Daniela Ioniţă, Elena Berteanu, Luminiţa Tcacenco, Adina Zuav and Ioana Demetrescu

Graphical Abstract
New membranes have been elaborated and their physicochemical properties were assessed. The water absorption permitted the evaluation of the diffusion coefficient and the enhancement of antibacterial activity and hemolytic properties was emphasized



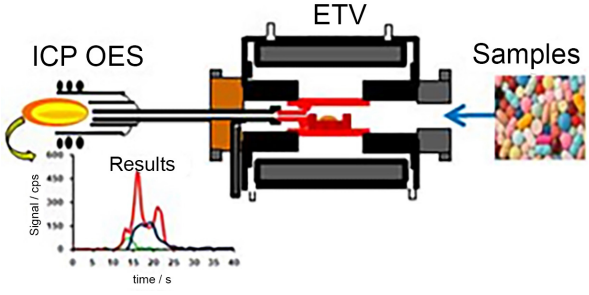
466 **A Prompt, Tough and Eco-Friendly (PTOCO) System for Mini-Scale Extraction of Samples for Antioxidant Capacity Assays**
Thiago Claus, Oscar O. Santos Júnior, Janksyn Bertozzi, Swami A. Maruyama, Sylvio V. Palombini, Eduardo J. Pilau, Carlos A. P. da Camara, Makoto Matsushita and Jesuí V. Visentainer

Graphical Abstract
The PTOCO (P = Prompt, TO = TOugh and CO = eCO-friendly) system of mini-scale antioxidant compounds extraction attends the need of obtain extracts in sufficient amounts for rapid and efficient application at several analytical methods, turning the routine of analysis in something more enjoyable



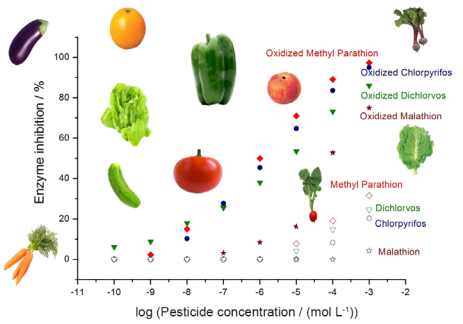
475 **Element Determination in Pharmaceuticals Using Direct Solid Analysis-Electrothermal Vaporization Inductively Coupled Plasma Optical Emission Spectrometry**
Suelem Kaczala, Adilson B. Costa, Ederson L. Posselt, Juliano S. Barin, Erico M. M. Flores and Valderi L. Dressler

Graphical Abstract
A solid sampling electrothermal vaporization inductively coupled plasma optical emission spectrometry (ETV-ICP OES) method was developed for element determination in pharmaceuticals



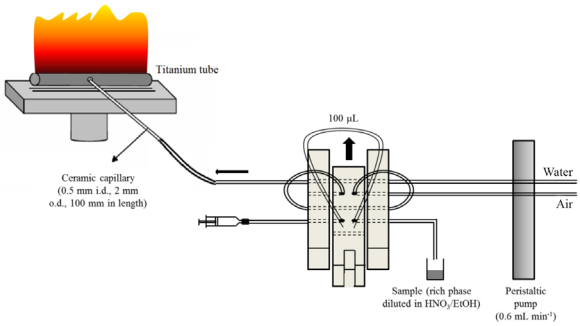
484 **Flow Injection Analysis System for Screening Organophosphorus Pesticides by their Inhibitory Effect on the Enzyme Acethylcholinesterase**
Marcos P. Silva, Matthieu Tubino, Tereza C. R. Elsholz, Olaf Elsholz, Sabir Khan and Marta M. D. C. Vila

Graphical Abstract
A flow-injection spectrophotometric procedure was developed for screening organophosphorus pesticides. The method is based on the inhibition of acetylcholinesterase immobilized on controlled porous glass beads with acetylcholine chloride as the substrate



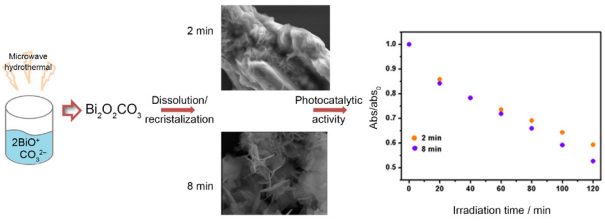
490 **Cadmium and Lead Determination in Freshwater and Hemodialysis Solutions by Thermospray Flame Furnace Atomic Absorption Spectrometry Following Cloud Point Extraction**
SI online
Samara Garcia, Fabiana Gerondi, Thiago R. L. C. Paixão, Marco A. Z. Arruda and Ivanise Gaubeur

Graphical Abstract
A procedure of sequential trace-level Cd and Pb determination by thermospray flame furnace atomic absorption spectrometry, after cloud point extraction, was developed. The proposed method presents high sensibility, low reagent consumption and reduced waste disposal



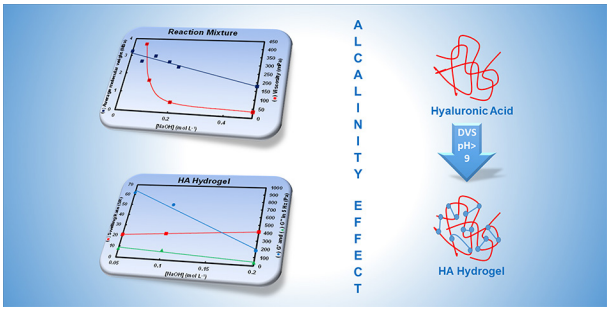
498 **Rapid Preparation of $(BiO)_2CO_3$ Nanosheets by Microwave-Assisted Hydrothermal Method with Promising Photocatalytic Activity Under UV-Vis Light**
SI online
Juliane Z. Marinho, Lidiaine M. Santos, Leilane R. Macario, Elson Longo, Antonio E. H. Machado, Antonio O. T. Patrocinio and Renata C. Lima

Graphical Abstract
$(BiO)_2CO_3$ nanosheets have been successfully prepared by a rapid reaction using the hydrothermal method combined with microwave heating. The as prepared $(BiO)_2CO_3$ nanosheets presented good photocatalytic activity for degradation of organic dye Ponceau P4R under UV-Vis light



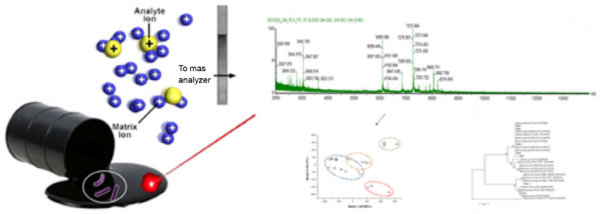
506 **The Performance of Crosslinking with Divinyl Sulfone as Controlled by the Interplay Between the Chemical Modification and Conformation of Hyaluronic Acid**
Andréa A. M. Shimojo, Aline M. B. Pires, Rafael Lichy and Maria H. A. Santana

Graphical Abstract
The effects of the alkaline medium of the reaction mixture on the swelling and rheological properties of hyaluronic acid (HA) microparticles crosslinked with divinyl sulfone with regard to the interplay between the HA conformation and the extension of the crosslinking reaction



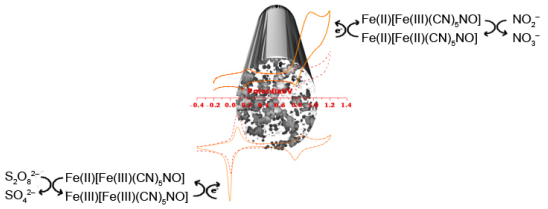
513 **Classification and Identification of Petroleum Microorganisms by MALDI-TOF Mass Spectrometry**
Célio F. F. Angolini, Eduardo J. Pilau, Patrícia F. Lopes-Oliveira, Isabel N. S. Garcia, Fábio C. Gozzo, Valéria M. de Oliveira and Anita J. Marsaioli

SI online



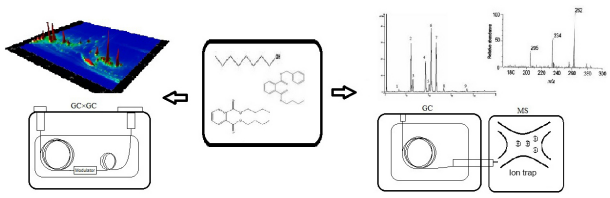
Graphical Abstract
Indigenous bacteria isolated from a crude oil sample were successfully classified in groups which match exactly with molecular identification using the *gyr*B gene sequence, showing the advantages of using this technique to build petroleum bacteria database

521 **Size Reduced Iron Nitroprusside Particles: an Electrochemical Mediator for the Quantification of Peroxodisulfate and Nitrite**
Samrat Devaramani, Ramakrishnappa Thippeswamy and Nathan S. Lawrence



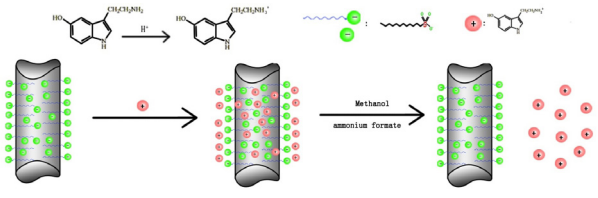
Graphical Abstract
Size reduced iron nitroprusside particles modified carbon paste electrode has been used for the electrochemical oxidation and reduction of NO_2^- and $S_2O_8^{2-}$ respectively

531 **Quantitative Analysis of Endocrine Disruptors by Comprehensive Two-Dimensional Gas Chromatography**
Miriany A. Moreira, Leiliane C. André, Alexandra B. Ribeiro, Marco D. R. G. da Silva and Zenilda L. Cardeal



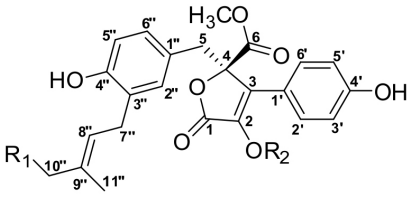
Graphical Abstract
The graphical abstract exemplifies the comparison between two methods of gas chromatography

537 **An Ion-Pair Reagent Incorporated Polystyrene Nanofiber Applied to Solid Phase Extraction of 5-Hydroxytryptamine in Human Plasma**
Yu Wang, Xiaoling Zhou, Yuqin Ma and Xuejun Kang



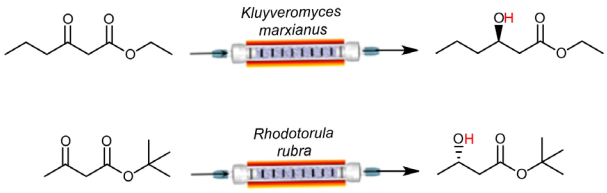
Graphical Abstract
Sodium dodecyl sulfonate incorporated polystyrene electrospun nanofibers was prepared and applied in ion exchange solid phase extraction

545 **Butyrolactones from the Endophytic Fungus *Aspergillus versicolor* and their Anti-Tobacco Mosaic Virus Activity**
Min Zhou, Jie Lou, Yin-Ke Li, Yue-De Wang, Kun Zhou, Bing-Kun Ji, Wei Dong, Xue-Mei Gao, Gang Du and Qiu-Fen Hu
SI online



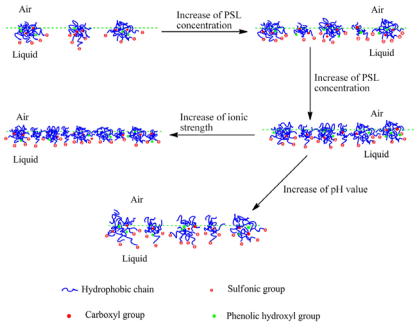
Graphical Abstract
New butyrolactones aspernolides C and D isolated from *Aspergillus versicolor*

550 **Improving the Toolbox of Bioreductions by the Use of Continuous Flow Systems**
Raquel O. Lopes, Simon Grimm, Joyce B. Ribeiro, Ivana C. R. Leal, Leandro S. M. Miranda and Rodrigo O. M. A. de Souza
SI online



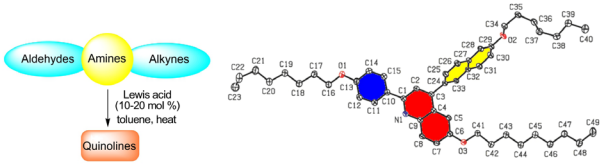
Graphical Abstract
This report showed the bioreduction of ethyl 3-oxohexanoate by immobilized *Kluyveromyces marxianus* cells and *tert*-butyl 3-oxobutanoate by immobilized *Rhodotorula rubra* cells under continuous flow conditions leading to the desired β-hydroxy esters corresponding in high yields and enantiomeric excess

555 **Adsorption Mechanism of Lignosulfonate at the Air/Liquid Interface**
Mingfang Yan and Dongjie Yang



Graphical Abstract
The configuration of PSL at the air/liquid interface will change from disorder to regularly as the concentration of PSL and the ionic strength of solution increase, but it will array from tightly to loose as the pH value of solution increases

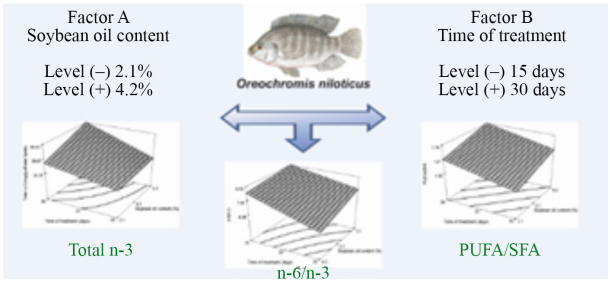
562 **Quinolines by Three-Component Reaction: Synthesis and Photophysical Studies**
Eric S. Sales, Juliana M. F. M. Schneider, Marcos J. L. Santos, Adailton J. Bortoluzzi, Daniel R. Cardoso, Willy G. Santos and Aloir A. Merlo
SI online



Graphical Abstract
Quinolines were synthesised by three-component reaction using Fe(III) and Yb(III) catalysts. From a single-crystal X-ray analysis for a synthesised quinolone, quinolyl and naphtyl groups connected to the C3 and C24 carbon atoms are twisted by torsion angle of 65.2°

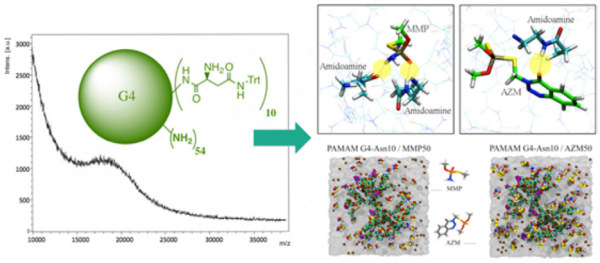
572 **Levels of Soybean Oil and Time of Treatment for Nile Tilapia: a Factorial Design for Total n-3 Fatty Acids, n-6/n-3 and PUFA/SFA Ratios**
Ana P. Lopes, Vanessa V. A. Schneider, Paula F. Montanher, Ingrid L. Figueiredo, Hevelyse M. C. Santos, Swami A. Maruyama, Angela M. M. Araújo and Jesuí V. Visentainer

Graphical Abstract
Response surfaces were obtained from a 2^2 factorial design for total n-3 fatty acids and n-6/n-3 and polyunsaturated fatty acids (PUFA)/saturated fatty acids (SFA) ratios in lipids of Nile tilapia fed with diets containing soybean oil



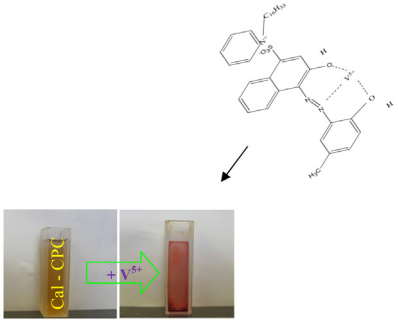
580 **Nano-Detoxification of Organophosphate Agents by PAMAM Derivatives**
SI online
Esteban F. Durán-Lara, Fabian Ávila-Salas, Sebastian Galaz, Amalraj John, Adolfo Maricán, Margarita Gutiérrez, Fabiane M. Nachtigall, Fernando D. Gonzalez-Nilo and Leonardo S. Santos

Graphical Abstract
Polyamidoamine (PAMAM) derivatives showed in *in vitro* studies the ability to capture methamidophos efficiently and could be used as an antidote to maintain acetylcholinesterase activity in poisoning events



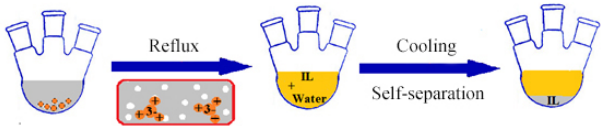
592 **Developing Fast and Facile Method for Speciation Analysis of Vanadium (V/IV) Ions with Calmagite Immobilization on Triacetyl Cellulose Membrane in Water Samples**
Hossein Tavallali and Rozita Nejabat

Graphical Abstract
The first speciation of V(VI/V) ions with optical sensor, which is more superior in terms of sensitivity and simplicity



600 **Optimization of Process Variables in the Synthesis of Isoamyl Isovalerate Using Sulfonated Organic Heteropolyacid Salts as Catalysts**
Keke Chen, Wei Yan, Xiaofang Zhang, Yingying Kuang, Xiujuan Tang and Xiaoxiang Han

Graphical Abstract
Sulfonated organic heteropolyacid salts with superior esterification rate, excellent durability, and unique self-separation property desirable for facile recovery and recycling during homogeneous synthesis of isoamyl isovalerate are reported

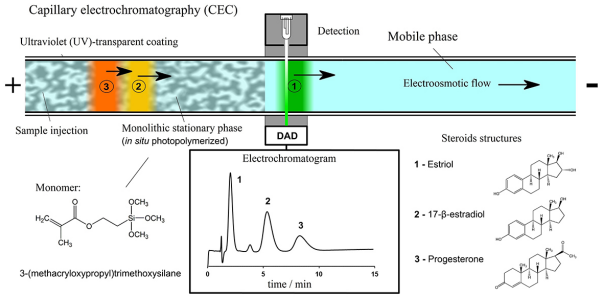


609 Optimized Separation Method for Estriol, 17-β-Estradiol and Progesterone by Capillary Electrochromatography with Monolithic Column and its Application to a Transdermal Emulsion

Rafael Marques, Fernando A. S. Vaz, Hudson C. Polonini and Marcone A. L. de Oliveira

Graphical Abstract

A 2^3 factorial design was employed to optimize separation between estriol, 17-β-estradiol and progesterone by capillary electrochromatography through a monolithic column based on 3-(methacryloxypropyl) trimethoxysilane monomer. Once optimized, the method was applied to the quantitative analysis of a transdermal emulsion



619 QSAR Study of the Inhibitors of the Acetyl-CoA Carboxylase 1 and 2 using Bayesian Regularized Genetic Neural Networks: A Comparative Study

SI online

Abolfazl Valadkhani, Mohammad Asadollahi-Baboli and Ahmad Mani-Varnosfaderani

Graphical Abstract

The Monte-Carlo sampling strategy was implemented in Bayesian regularized genetic neural network (BRGNN) algorithm for quantitative structure-activity relationship modeling of acetyl-CoA carboxylase (ACC) inhibitors. The calculated activities using BRGNN algorithm in this work are in good agreement with experimental values. The results of the present work emphasizes on the role of positive charge and polarity of molecules on ACC inhibitory activity